Competing supersolids of ultracold Bose-Bose mixtures in a triangular optical lattice

Fabien Trousselet,[1] Pamela Rueda,[2] and Arnaud Ralko[1]

[1] *Institut Néel, UPR-2940, CNRS et Université Joseph Fourier, Grenoble, F-38042 France*
[2]*INAC-SP2M, CEA et Université Joseph Fourier , Grenoble, FR-38054, France*
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We study the ground state properties of a frustrated two-species mixture of bosons in an optical triangular lattice, as a function of tunable amplitudes for tunnelling and interactions. By combining three different methods, a self-consistent cluster mean-field, exact diagonalizations and effective theories, we unravel a very rich and complex phase diagram. More specifically, we discuss the existence of three original mixture supersolids: (i) a commensurate with frozen densities and spin-like *color* supersolidity, in a regime of strong interspecies interactions; and (ii) when this interaction is weaker, two mutually competing incommensurate supersolids. Finally, we show how these phases can be stabilized by the quantum melting of peculiar insulating parent Mott states.

Ultracold atoms on optical lattices form one of the most fascinating fields of research in nowadays condensed matter physics. These systems are highly versatile, thanks to the possibilities to control the lattice dimension and geometry, the statistics of loaded atoms, their mutual interactions, as well as to create atom mixtures. Therefore, an incredible amount of exotic phases has been reported in the literature these last years, both experimental and theoretical, such as unconventional Mott insulators, superfluids [1], Bose metals [2–4] or supersolid phases. In this last case, the system enters a phase combining both crystalline order and superfluidity, and typically arising from the quantum melting of a Mott insulator; this phenomenon is at the origin of intense scientific activities and debates. Experimentally, supersolidity is expected to be realized in solid ^{4}He [5], but necessary conditions for continuous symmetry breaking led to question this observation [6], which was eventually contradicted by more recent experiments [7]. However, supersolids are easier achieved on lattice systems; whereas on a square geometry with nearest neighbor interactions a soft-core description is required [8], they can also be found in hard-core bosonic models when frustration is induced by either further neighbor interactions [9] and/or lattice geometry, *e.g.* triangular [10–12]. In this context, the recent progress in optical lattice engineering gives good hopes for observing supersolidity on non-bipartite lattices [13, 14]. One of the most promising directions is the study of mixtures, in particular those with several species of bosons, either heteronuclear as ^{41}K-^{87}Rb [15] or homonuclear with two different spin states, e.g. $|1,-1\rangle$ and $|2,-2\rangle$ states of ^{87}Rb [16]. Another way to realize mixtures is to consider, as we will do in this paper, bilayer systems with interactions but no hopping between layers [17]. Such systems allow for an even broader variety (compared to single-species counterparts) of quantum phases, depending on the intra- and inter-species interactions, and on the dimension and lattice connectivity. Compared to an already rich literature on mixtures in 1D (*e.g.* [18]) only few works have focused on 2D cases, for instance on square [19] and triangular [20–22] lattices. In all those systems, contact and dipolar interactions [17, 23, 24] can be tuned using Feshbach resonances and by an external electric field [25] respectively. Since both interactions, considered independently, tend to favor different types of Mott insulators, *e.g.* density-homogeneous or density wave [26], the competition between both can, along with quantum fluctuations, trigger various unconventional phases [10, 17, 24], especially on frustrated lattices.

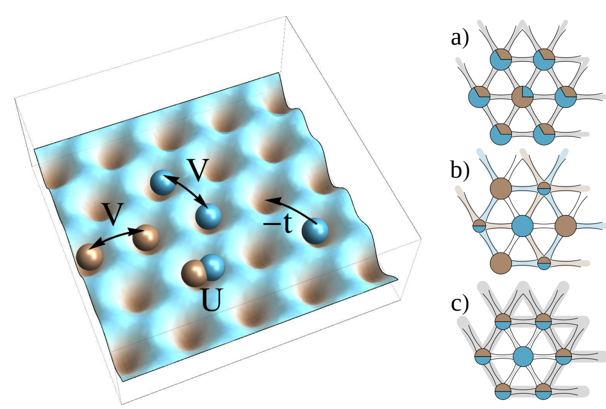

FIG. 1: Left: Triangular optical bilayer lattice as can be realized by a set of laser beams, and hosting two types of bosons labelled a (blue) and b (brown). Right: Sketch of the two-component supersolids with 3-sublattice structure: (a) the $n = 1$ spin-like *color* supersolid (CSS), (b) the 3-supersolid (3SS); and (c) the bosonic pinball (BPB), all described in the text. The larger the disc, the higher the density.

In this Letter, we study bosons loaded in an optical bilayer triangular lattice, or equivalently a two-color (species) bosonic mixture on a monolayer (see Fig. 1). The richness of the phase diagram of the bosonic extended Hubbard model on the triangular lattice, specifically with hard core constraint [12], allows us to expect even more exotic physics when the inter-color interactions are switched on. Indeed, these can mimic efficiently the frustrating effects of dipolar couplings that can arise in cold atom systems [10, 12, 17], whereas further range

interactions have minor effects in the corresponding density regimes. Here, we address the following issues: (i) how lattice frustration impacts on the stabilization of non-conventional phases of such mixture and (ii) how on-site and nearest neighbor interactions compete. To achieve these goals, we use *cluster mean field* theory (CMFT) and exact diagonalizations (ED) on periodic clusters, as well as perturbative approaches. The former method has been employed successfully in many one-component bosonic systems on various lattices such as triangular [12, 26, 31], Cairo-pentagonal [27] and hexagonal [28]. It is thus expected to be also very efficient in the present two-component(bilayer) model. Our main findings are the presence of three original two-component supersolid (SS) phases: two incommensurate with density modulations, and one commensurate with frozen densities and spin-like color supersolidity.

Model and method– We study a two-component extended Bose-Hubbard model on a triangular lattice:

$$
\begin{aligned}
H_\alpha &= \sum_{\langle i,j\rangle} \left[-t_\alpha(b^\dagger_{i\alpha}b_{j\alpha}+h.c.)+V_\alpha n_{i\alpha}n_{j\alpha}\right]-\mu_\alpha\sum_i n_{i\alpha}\\
H_{ab} &= \sum_\alpha H_\alpha + U\sum_i n_{ia}n_{ib}. \qquad (1)
\end{aligned}
$$

equivalent to a one-component bosons on a bilayer triangular lattice since no inter-site/inter-color couplings is considered. H_α is the one-color Hamiltonian ($\alpha = a/b$), with μ_α the chemical potential, t_α and V_α respectively the nearest neighbor hopping and interaction amplitudes. For consistency, an extra term $U_{\alpha\alpha}\sum_i n_{i\alpha}(n_{i\alpha}-1)/2$ describing the on-site repulsion between bosons of same color (soft core) has to be included in H_α. However, we are primarily interested in the effects of frustration induced by inter color couplings U. These are typically reached in the strong interaction limit where the dominant coupling $U_{\alpha\alpha}$ imposes hard core constaints $n_{i\alpha}\leq 1$. All the phases reported in this paper can be stabilized for $U_{\alpha\alpha}\gtrsim 3V$; from now on, $b^\dagger_{i\alpha}$ is the creation operator of a hard core boson of color α at site i. In addition, by sampling the parameter space, we found that the most original two-component phases arise when the system is a/b-symmetric ($t_\alpha = t$, $V_\alpha = V$ and $\mu_\alpha = \mu$) [29]. This case, considered in this work, allows by the particle-hole canonical transformation $b'_{i\alpha} = b^\dagger_{i\alpha}$ the use of a mapping between cases $\mu^* > 0$ and $\mu^* < 0$, with $\mu^* = \mu-3V-U/2$ a rescaled chemical potential.

We compute the ground states of H_{ab} on clusters up to $N = 12$ sites by either ED or CMFT methods. In the latter case, the N_i (N_e) internal (external) bonds are treated exactly (at the mean field level). See Refs. [12, 30, 31] for more details. The mean-field parameters determined self-consistently are the densities $\bar{n}_{i\alpha} = \langle n_{i\alpha}\rangle$ and the superfluid fractions (SF) $\phi_{i\alpha} = \langle b_{i\alpha}\rangle$. In addition, to evidence 3-fold symmetry breaking, we define the order parameter $M_\alpha = |\bar{n}_\alpha(k)|$ and the color-color correlation function $S_{ab} = |\langle(n_a-n_b)(-k)(n_a-n_b)(k)\rangle|^2$. We used the Fourier transform $n_\alpha(k) = \frac{1}{N}\sum_s n_{s\alpha}e^{ik\cdot r_s}$ at point $k = (4\pi/3, 0)$, corner of the Brillouin zone. As in Ref. [31], we define the scaling parameter $\lambda = N_i/(3N)$ which quantifies finite boundary effects. Hence, the Thermodynamic Limit (TL) is achieved for $\lambda \to 1$ (infinite lattice).

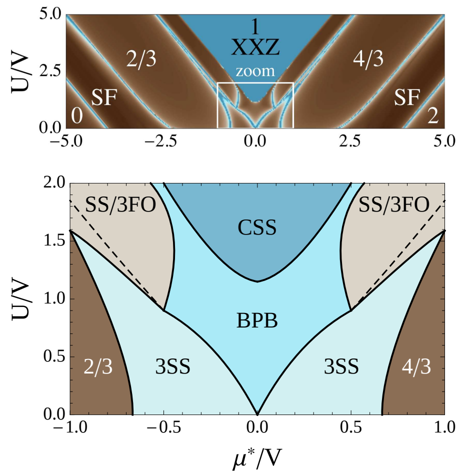

FIG. 2: Phase diagrams as obtained from CMFT calculations on a $N = 3$ cluster at $t = 0.15$ and $V = 1$. Top: Complete range of μ^* showing two-component superfluids, 2/3 and 4/3 plateaus, XXZ physics domain and pure two-component physics not reminiscent to the phases of the one-specie boson system (white rectangle). Bottom: zoom of the white rectangle and all new two-component phases (see text for acronyms). Solid (dashed) lines are phase boundaries subsisting (vanishing) in the Thermodynamic Limit (TL).

Overview of the phase diagram– Let us first focus on the (μ^*, U) phase diagram in which novel two-color phases - detailed along the paper - emerge, illustrated here for $t/V = 0.15$. For these parameters, the one-color Hamiltonian H_α is known to present a rich phase diagram with either empty/full, homogeneous superfluid, $\sqrt{3}\times\sqrt{3}$ solid at density 1/3 or supersolid phases [10]. When U is switched on, the correlations between the two colors increase, and resulting GS can be either a product of two one-color phases or color-entangled states as depicted in the complete phase diagram shown in Fig. 2. (i) As $\mu^* < 0$ increases, the first non-trivial phase encountered is a homogeneous two-color superfluid with $\phi_a = \phi_b \neq 0$ ($\phi_\alpha = \frac{1}{N}\sum_i \phi_{i\alpha}$). When n_a and n_b are high enough, V and U terms become costful and the system enters a 3-fold ordered insulator characterized by $\phi_a = \phi_b = 0$ and a total density $n = 2/3$ ($n_a = n_b = 1/3$), the two-color counterpart of the $\sqrt{3}\times\sqrt{3}$ phase. (ii) At even larger density, various supersolids with 3-sublattice structures are stabilized. Finally, a phase with $n = 1$ is stabilized for $U > 1.2V$. For $\mu^* > 0$, we obtain an equivalent phase diagram thanks to the particle-hole symmetry. The most original of these two-color phases are detailed hereafter.

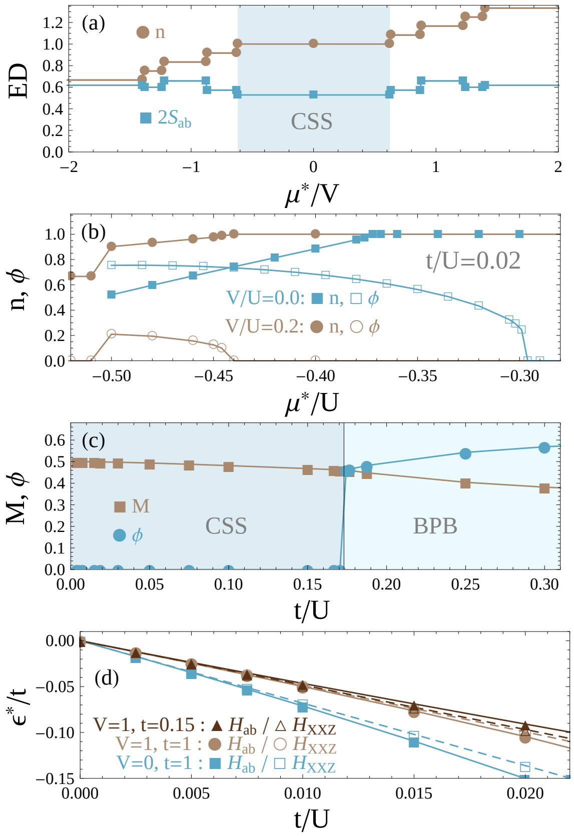

FIG. 3: Strong U regime characterized using either $N = 12$ (ED: a,d) and $N = 6$ (CMFT: b,c) clusters. (a) n and S_{ab} as a function of μ^*/V for $U = 2V$ and $t = 0.15V$. The $n = 1$ plateau and the finite S_{ab} evidence the CSS; (b) n and $\phi = \phi_a + \phi_b$ as a function of μ^*/U distinguishing the CSF ($V = 0$) and the CSS ($V = 0.2U$) regimes; (c) quantum melting of the CSS to the BPB phase (see text); (d) comparison of the kinetic energy gain $\epsilon^* \simeq -kt^2/U$ for H_{ab} (filled) and $H_{\rm XXZ}$ (empty) for three (t, V) sets.

Commensurate spin-like phases– For strong inter-color repulsion $U \gg V, t, |\mu^*|$ (triangular uppermost domain on Fig. 2-up) the system is Mott insulating, with $\phi_\alpha = 0$ and $n = 1$. Indeed, U imposes the local constraint of single occupancy defined as $n_a + n_b = 1$. This is reflected in ED by the $n = 1$ plateau on Fig. 3(a,b) and in CMFT by the $n_\alpha = 1/2$ plateau on Fig. 4(right). In order to better describe this regime, we define spin 1/2 operators $\sigma_i^z = (n_{ia} - n_{ib})/2$ and $\sigma_i^+ = b_{ia}^\dagger b_{ib}$. At second order of the perturbation theory, we obtain an effective XXZ model

$$H_{\rm XXZ} = -\frac{J_\perp}{2} \sum_{\langle i,j \rangle} (\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+) + J_z \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z, \quad (2)$$

where $J_\perp = 4t^2/U$ and $J_z = 2V + 4t^2/U$. Interestingly, this model predicts a $(2m_z, -m_z, -m_z)$ SS with diagonal $\langle \sigma^z \rangle \neq 0$ and off-diagonal $\langle \sigma^+ \rangle \neq 0$ order parameters when $J_z/J_\perp > 4.6(1)$; otherwise, a SF with only off-diagonal order [32, 33]. In the present context, these phases correspond respectively to a *color supersolid* (CSS) and a *color superfluid* (CSF). While the density is uniform, the CSS has a $(2m_z, -m_z, -m_z)$ structure where m_z quantifies the color disproportion on each sublattice. As depicted in Fig. 3, for $|\mu^*| \ll V$, both ED and CMFT are consistent with the CSS scenario; indeed the finite structure factor S_{ab} and $M = (M_a + M_b)/2$ for $t/U < 0.17$ signal long-range correlations and the corresponding XXZ couplings verify $J_z/J_\perp = 1 + UV/2t^2 \geq 20.5$. In contrast, for $V = 0$ and $t/U \leq (t/U)_c \simeq 0.05(1)$ we find in vicinity of $\mu^* = 0$ the spatially uniform *CSF* predicted in the XXZ model, as illustrated in Fig. 3(b). Finally, Fig. 3(d) shows that the kinetic energy gain $\epsilon^* \simeq -kt^2/U$ w.r.t. the electrostatic contribution $N(V - \mu)$ is well reproduced by the XXZ model in both regimes; this validates our approach.

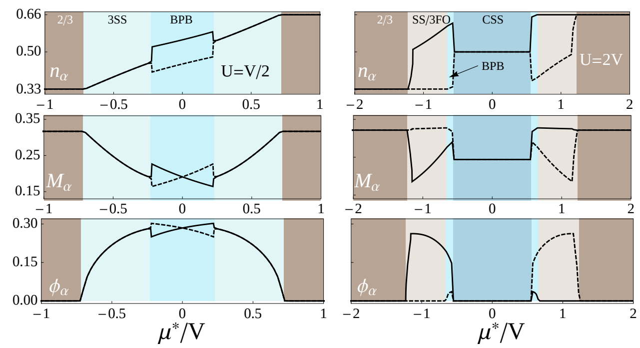

FIG. 4: Color-resolved observables $(n_\alpha, M_\alpha, \phi_\alpha)$. Each color corresponds to either continuous or dashed line. All data come from a $N = 6$ CMFT with fixed $t/V = 0.15$ and $U = 0.5V$ (left) or $2V$ (right). The arrow points out a tiny region which disappears in the TL (see text). The shaded regions correspond to the different phases of Fig. 1.

Incommensurate supersolids– In contrast to the above mentioned CSS in which supersolidity comes from the color spin-like degrees of freedom, in SS phases discussed here n_α may be incommensurate and they have finite ϕ_α. From the color-resolved observables shown in Fig. 4, we identify three such SS phases. (i) For large $U/V = 2$ (right column) and μ^*/V about $\pm 1.0(2)$, the finite M_α indicates a 3-fold order (3FO) for both colors, while only one component has a non-zero ϕ_α. This phase, dubbed SS/3FO in Fig. 2, is a rearrangement of two one-color phases of H_α, the $\sqrt{3} \times \sqrt{3}$ solid and the SS obtained from its melting [10, 12]. Two sublattices are (almost) filled by a and b bosons respectively, while on the remaining, an incommensurate density for bosons of one color accounts for superfluidity. Within this structure, the repulsion energy $\propto U$ is minimized thanks to the localization of bosons of a single color. (ii) For small $U/V = 0.5$ (left column) and μ^*/V about $\pm 0.5(3)$, the phase has a finite ϕ_α for both colors as well as a 3-fold symmetry

breaking. This phase, called 3-fold SS (3SS) is the first example of a collective two-color supersolid. As shown in Fig. 1(b), it can be seen as a superposition of two one-color SS (these would be obtained at $U = 0$); both colors contribute symmetrically to superfluidity. Note that this 3SS is obtained from the parent $n = 2/3$ solid by a defect condensation upon doping as μ^* increases. As in this parent state, the weak inter-color coupling merely forces the localized a and b bosons to occupy distinct sublattices. (iii) The most remarkable incommensurate SS phase is achieved by the quantum melting of the density-uniform $n = 1$ CSS. This original two-color SS is called the *bosonic pinball* (BPB) due to a structure very similar to its fermionic counterpart with similar interactions, the *pinball liquid*. It has almost one localized electron per site on one sublattice (pins) and a metallic behavior on the remaining hexagonal lattice (balls) [26, 34, 35]. Here, the particles are bosonic and the colors play the role of the spins. The structure is depicted on Fig.1(c). One sublattice, forming a triangular super-lattice with $\bar{n}_{ia} + \bar{n}_{ib}$ are close to 1, is filled in majority by one type of bosons. The two-color superfluid character is carried by the remaining bosons on the complementary hexagonal lattice. This is shown in the BPB region on Fig. 4(left column) and Fig. 5, by a coexistence of a solid $M_\alpha \neq 0$ and superfluid $\phi_\alpha \neq 0$ orders in both colors. This lattice symmetry breaking is reminiscent of the parent CSS phase, the quantum melting of which involves a condensation of two types of defects coming from doubly-occupied and empty sites. Finally, unlike the 3SS and SS/3FO, the BPB can be stabilized at the $n = 1$ commensurability when $\mu^* = 0$. In Fig. 5 are displayed the cluster dependency of M and ϕ for two examples illustrating the BPB and the 3SS which confirms their existence at the TL as $\lambda \to 1$ (inset).

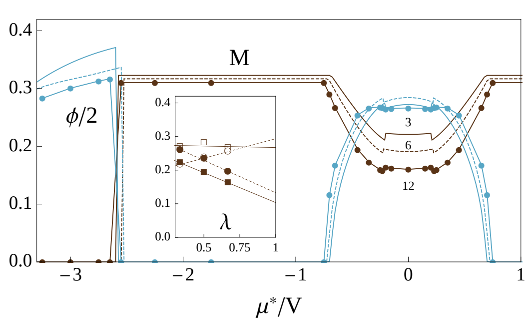

FIG. 5: M and ϕ as a function of μ^* for $t = 0.15V$ and $U = 0.5V$ obtained by CMFT on clusters of $N = 3$ (continuous), 6 (dashed) and 12 (symbols) sites. (Inset) cluster scaling as function of λ (see text) of M (filled symbols) and $\phi/2$ (empty symbols), for the BPB at $|\mu^*| = t$ (squares) and the 3SS at $|\mu^*| = 3t$ (circles).

Phase transitions– We checked that the phase boundaries are only weakly affected by size effects. The phase diagram of Fig. 2 is then representative of the TL. It is possible to extract an estimate of certain of these transitions when defects proliferate as their energy cost vanish (condensation picture), in the strong correlation limit $U, V \gg t$ [36], as it is the case for the $2/3 \to$ 3SS transition. Consider a defect consisting of an extra boson (say of color a) inserted in the *empty* sublattice of the $2/3$ crystal with the energy cost $3V$. Via second order processes, such a defect can hop to second neighbors with an amplitude $-t_{\text{eff}} = -t^2/U - t^2/V$ [37]. In this limit, the defects condense and lead to supersolidity for $\mu_c = 3V - 6t_{\text{eff}}$, *e.g.* $\mu_c/V \simeq -0.65$ for $U = 0.5V$ in good agreement with the results of Fig. 4. This defect condensation mechanism implies a gauge symmetry breaking additionally to the already broken lattice symmetry of the $2/3$ phase. This indicates that the transition is of second order, as confirmed by the absence of discontinuities in ϕ and M as function of μ (Fig. 5). This corresponds to the standard picture of defect condensation accounting for an incommensurate SS; the SF density (here inhomogeneous) is carried by defects on top of density modulations [10]. In contrast, the transitions between (i) homogeneous SF and $2/3$ solid, and (ii) the BPB and 3SS are found of first order, characterized by hysteresis in the CMFT [38]. In case (ii) for example, 3SS and BPB have distinct broken symmetries as displayed in Fig. 1(b,c).

Conclusions– We study interacting hard-core bosons in an optical bilayer triangular lattice equivalent to a two-color bosonic mixture on a monolayer, by combining both ED and CMFT methods. We focus on a region of parameter space in which novel phases arise due to the competition between frustration and quantum fluctuations. Within a very rich and complex phase diagram, we evidence three original mixture supersolids with 3-site unit cell structures: (i) a *spin-like* commensurate phase termed the *color supersolid* (CSS), characterized by an effective XXZ model with frozen densities and supersolidity carried by the color degrees of freedom. (ii) two mutually competing incommensurate phases arising from the quantum melting of parent states, either the 2/3-solid or the original CSS, via defect condensation mechanisms. Melting the $2/3$ phase leads to a *3-fold supersolid* (3SS) with three inequivalent sites. The most interesting supersolid comes from the melting of the CSS and directly results from strong effects of inter-color coupling. The inner structure of this *bosonic pinball* (BPB) is very reminiscent to that of its fermionic counterpart. These striking features found in the hard-core limit and by truncating long-range to n.n. interactions tunable experimentally, are expectable in a broader variety of situations (dipolar interactions, sot-core bosons) which should stimulate further investigations.

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